Abstract Submitted
for the DFD19 Meeting of
The American Physical Society

Natural gas supercritical properties: a multiscale molecular simulations study[1] ALEXSANDRO KIRCH, NAIYER RAZMARA, JULIO MENEGHINI, CAETANO MIRANDA, Universidade de São Paulo — A typical deficiency of continuum approach relies on the models describing averaged fluid properties. In particular, those models usually do not consider important molecular features occurring at the atomistic level, which influences the macroscopic regime. A suitable strategy to describe these phenomena occurring over temporal and spatial scales is to combine the continuum mechanics with higher resolution methodologies within a multiscale scheme. In this context, molecular dynamics (MD) simulations provide reliable values to describe fluid basic properties. The obtained quantities could serve as input parameters to address multiscale issues observed in numerous scientific and industrial applications, including the Oil Gas challenges. In present study, we take advantage of the predictive role handled by MD simulations to determine natural gas properties in the supercritical region, since there exist a lack of experimental data describing the mixture properties. In light of the multiscale approach, we discuss how the gas density, viscosity, and diffusion could feed lower resolution methodologies to address Oil Gas interest systems, including nanoflows in porous media and membranes technology for gas separation.

[1]The authors acknowledge the sponsorship of the Research Centre for Gas Innovation (FAPESP Proc. 2014/50.279-4) and SHELL Brasil.

Alexsandro Kirch
Universidade de São Paulo

Date submitted: 02 Aug 2019 Electronic form version 1.4